

UT-BATTELLE

Color Symmetry and Magnetic Space Groups

Bryan C. Chakoumakos

Center for Neutron Scattering
Oak Ridge National Laboratory,
Oak Ridge, Tennessee 37831-6393
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- Symmetry groups
- History- bicolor symmetry
- Anti-symmetry operations
- bicolor point groups
- Magnetic space groups
- Cosets
- Magnetic space group lattices
- Opechowski-Guccione symbols

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Group definition and properties

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

Associativity: For all a, b and c in G , $(a * b) * c = a * (b * c)$.

Identity element: There is an element e in G such that for all a in G , $e * a = a * e = a$.

Inverse element: For all a in G , there is an element b in G such that $a * b = b * a = e$, where e is the identity element from the previous axiom.

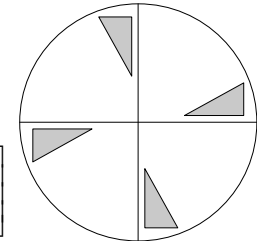
You will often also see the axiom:

Closure: For all a and b in G , $a * b$ belongs to G .

Example: Proper point group 4

$$4 = \{ 1, 4, 2, 4^{-1} \}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



Bicolor Symmetry Groups

1929 Heesch, introduces the antiidentity operation
properties: $u^2 = 1$, $ut = tu$ for all $t \in T$
aka time reversal group = $\{1, u\}$

1945 Shubnikov, re-introduces concept

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

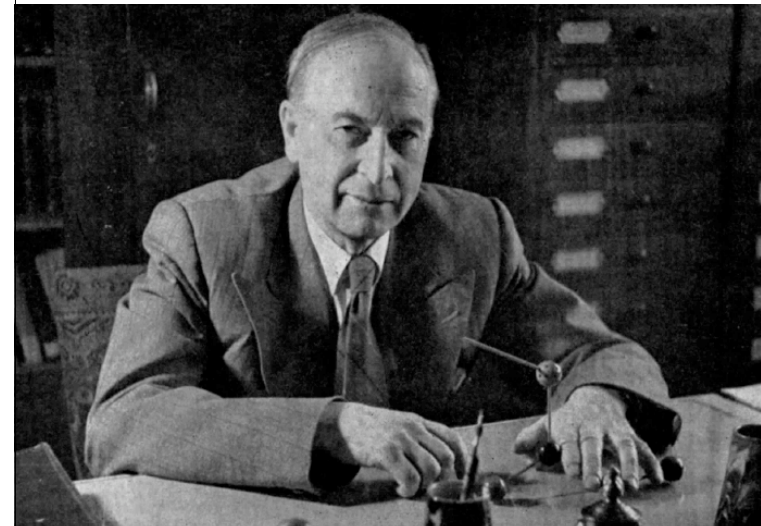
1955 Belov et al., first complete listing of the bicolor space groups

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



Daniel B. Litvin
 (1940-)
 Pennsylvania State University
<http://www.bk.psu.edu/faculty/Litvin/>



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

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

H	$2 = \{1, 2\}$	$m = \{1, m\}$	$\bar{1} = \{1, i\}$
$G \setminus H$	$\{i, m\}$	$\{2, i\}$	$\{2, m\}$
$(G \setminus H)1'$	$\{i', m'\}$	$\{2', i'\}$	$\{2', m'\}$
$H \cup (G \setminus H)1'$	$\{1, 2, i', m'\}$	$\{1, 2', i', m\}$	$\{1, 2', i', m'\}$
M	$2/m'$	$2'/m$	$2'/m'$

Example Magnetic Point Groups

Type I G	Type II G U Gu	Type II H U (G \setminus H)u
$2 = \{1, 2\}$	$21' = \{1, 2, 1', 2'\}$	$2' = \{1, 2'\}$
32 crystallographic point groups	32 crystallographic grey point groups	58 crystallographic Heesch point groups
122 crystallographic magnetic point groups		

Point group	nontrivial	magnetic	point	groups
1				
-1	-1'			
m	m'			
2	2'			
2/m	2'/m	2/m'	2'/m'	
222	2'2'2'			
mm2	m'm2'	m'm'2		
mmm	m'mm	m'm'm	m'm'm'	
4	4'			
-4	-4'			
4/m	4'/m	4/m'	4'/m'	
422	4'22'	42'2'		
4mm	4'm'm	4m'm'		
-42m	-4'2'm	-4'2'm'	-42'm'	
4/mmm	4'/m'mm	4'/mm'm	4'/m'm'm	4/mm'm'
3				

Point group	nontrivial	magnetic	point	groups	
-6	-6'				
32	32'				
3m	3m'				
-6m2	-6'm'2	-6'm2'	-6m'2'		
6	6'				
-3	-3'				
6/m	6'/m	6/m'	6'/m'		
622	6'2'2	62'2'			
6mm	6'm'm	6m'm'			
-3m	-3'm	-3m'	-3'm'		
6/mmm	6'/mmm	6'/mm'm	6'/m'm'm	6/mm'm'	6/m'm'm'
23					
m-3	m'-3				
-43m	-4'3m'				
432	4'32'				
m-3m	m'-3m	m-3m'	m'-3m'		

matrix representations of antisymmetry operations

4 X 4

$$\begin{bmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \bar{1} \end{bmatrix} \quad \begin{bmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & \bar{1} \end{bmatrix}$$

$^{[010]}2$ half-turn antiidentity $^{[010]}2'$ anti-half-turn

Seitz notation $(2_y|0,0,0)$ $(1|0,0,0)'$ $(2_y|0,0,0)'$

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
230 uncolored

Type II, $M = F \cup F1'$ for some crystallographic space group F
230 grey

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.

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 $a \in G$. Then the right coset of H in G determined by a, denoted Ha, is

$$Ha = \{ha \mid h \in H\}$$

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

$$aH = \{ah \mid h \in H\}$$

A subgroup H of a group G is said to be normal if $gH = Hg$ for all $g \in G$, 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 $g \in 4$.

$$\begin{aligned} 2*1 &= \{1, 2\}1 = \{1, 2\} & 1*2 &= 1\{1, 2\} = \{1, 2\} \\ 2*4 &= \{1, 2\}4 = \{4, 4^{-1}\} & 4*2 &= 4\{1, 2\} = \{4, 4^{-1}\} \\ 2*2 &= \{1, 2\}2 = \{2, 1\} & 2*2 &= 2\{1, 2\} = \{2, 1\} \\ 2*4^{-1} &= \{1, 2\}4^{-1} = \{4^{-1}, 4\} & 4^{-1}*2 &= \{1, 2\}4^{-1} = \{4^{-1}, 4\} \end{aligned}$$

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 $T = (I|t_j)$ 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 $(I|t_j)(W|w) = (W|w+t_j)$, 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

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Type II, $M = F \cup F1'$ 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)

$$F = P2/m = T(1|0,0,0) + T(2_y|0,0,0) + T(m_y|0,0,0) + T(i|0,0,0)$$

$$D = Pm = T(1|0,0,0) + T(m_y|0,0,0)$$

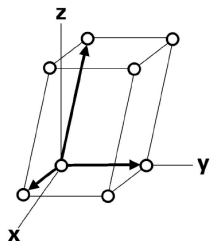
$$M_T = D + (F \setminus D)1'$$

$$(F \setminus D) = T(2_y|0,0,0) + T(i|0,0,0)$$

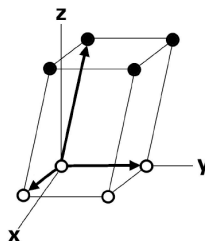
$$(F \setminus D)1' = T(2_y|0,0,0)' + T(i|0,0,0)'$$

$$M_T = T(1|0,0,0) + T(m_y|0,0,0) + T(2_y|0,0,0)' + T(i|0,0,0)'$$

MAGNETIC SPACE GROUP LATTICES triclinic system



$$P = P_{a,b,c}$$



$$P_{2s} = P_{a,b,2c}$$

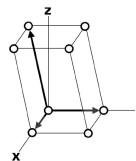
$$T_{\alpha} = c = (0,0,1)$$

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

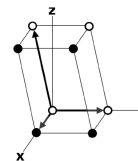
T_{α} = anti-translation

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

MAGNETIC SPACE GROUP LATTICES monoclinic system (y is the unique axis)

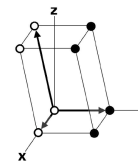


$$P = P_{a,b,c}$$



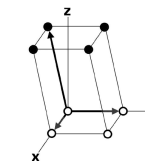
$$P_{2a} = P_{2a,b,c}$$

$$T_{\alpha} = a = (1,0,0)$$



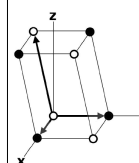
$$P_{2b} = P_{a,2b,c}$$

$$T_{\alpha} = b = (0,1,0)$$



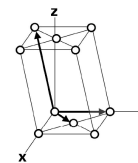
$$P_{2c} = P_{a,b,2c}$$

$$T_{\alpha} = c = (0,0,1)$$

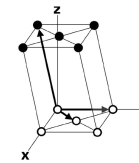


$$P_C = P_{2a,a+b,c} = P_{a-b,a+b,c}$$

$$T_{\alpha} = a = (1,0,0)$$

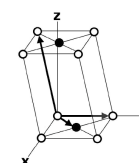


$$C = C_{\frac{1}{2}(a+b),b,c}$$



$$C_{2c} = C_{\frac{1}{2}(a+b),b,2c}$$

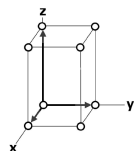
$$T_{\alpha} = c = (0,0,1)$$



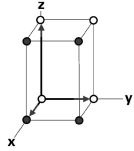
$$C_P = C_{a+b,b,c} = C_{a,b,c}$$

$$T_{\alpha} = \frac{1}{2}(a+b) = (\frac{1}{2}, \frac{1}{2}, 0)$$

MAGNETIC SPACE GROUP LATTICES orthorhombic system

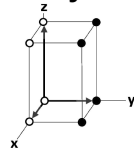


$$P = P_{a,b,c}$$



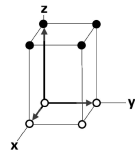
$$P_{2a} = P_{2a,b,c}$$

$$T_{\alpha} = a = (1,0,0)$$



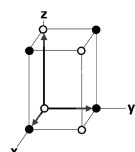
$$P_{2b} = P_{a,2b,c}$$

$$T_{\alpha} = b = (0,1,0)$$



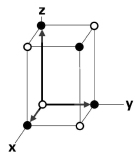
$$P_{2c} = P_{a,b,2c}$$

$$T_{\alpha} = c = (0,0,1)$$



$$P_C = P_{2a,a+b,c}$$

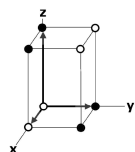
$$T_{\alpha} = a = (1,0,0)$$



$$P_F = P_{2a,a+b,c}$$

$$= P_{a+b,b+c,a+c}$$

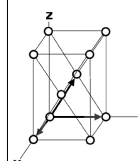
$$T_{\alpha} = a = (1,0,0)$$



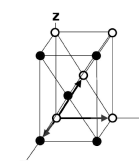
$$P_A = P_{a,2b,b+c}$$

$$T_{\alpha} = b = (0,1,0)$$

MAGNETIC SPACE GROUP LATTICES orthorhombic system, continued

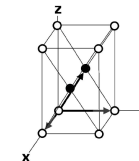


$$A = A_{a,b,\frac{1}{2}(b+c)}$$



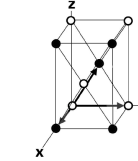
$$A_{2a} = A_{2a,b,b+c}$$

$$T_{\alpha} = a = (1,0,0)$$



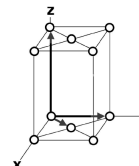
$$A_P = A_{a,b,c}$$

$$T_{\alpha} = \frac{1}{2}(b+c) = (0, \frac{1}{2}, \frac{1}{2})$$

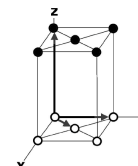


$$A_1 = A_{2a,b,\frac{1}{2}(2a+b+c)}$$

$$T_{\alpha} = a = (1,0,0)$$

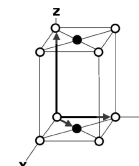


$$C = C_{\frac{1}{2}(a+b),b,c}$$



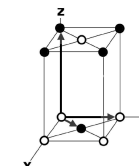
$$C_{2c} = C_{\frac{1}{2}(a+b),b,2c}$$

$$T_{\alpha} = c = (0,0,1)$$



$$C_P = C_{a+b,b,c} = C_{a,b,c}$$

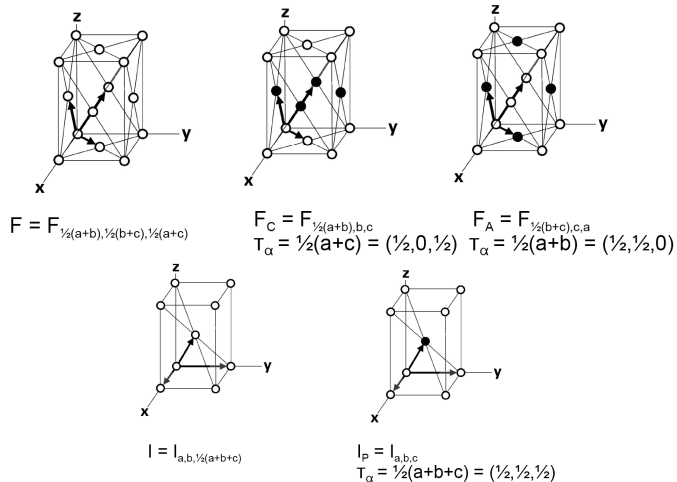
$$T_{\alpha} = \frac{1}{2}(a+b) = (\frac{1}{2}, \frac{1}{2}, 0)$$



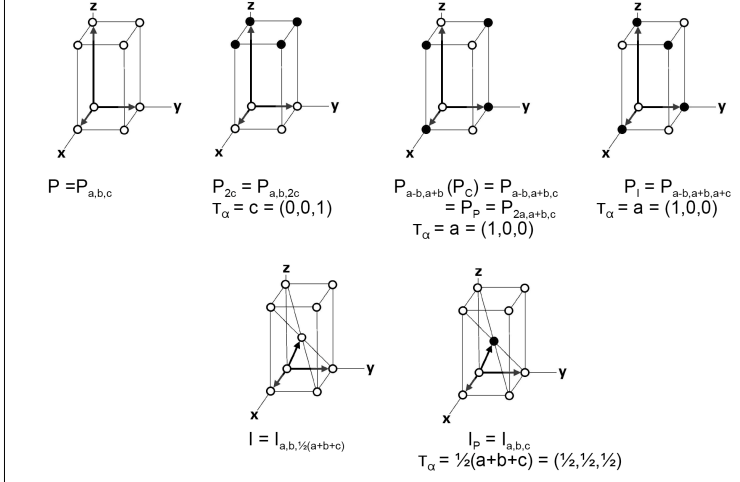
$$C_1 = C_{a,b,\frac{1}{2}(a+b+2c)}$$

$$T_{\alpha} = c = (0,0,1)$$

MAGNETIC SPACE GROUP LATTICES orthorhombic system, continued

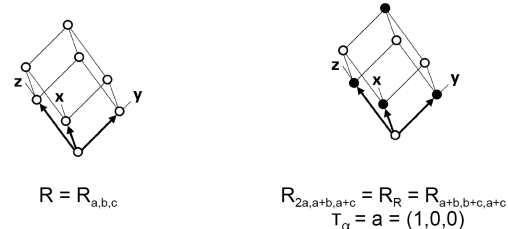


MAGNETIC SPACE GROUP LATTICES tetragonal system

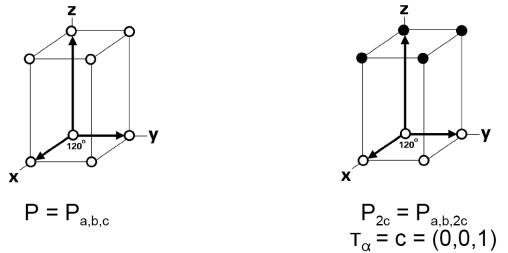


MAGNETIC SPACE GROUP LATTICES

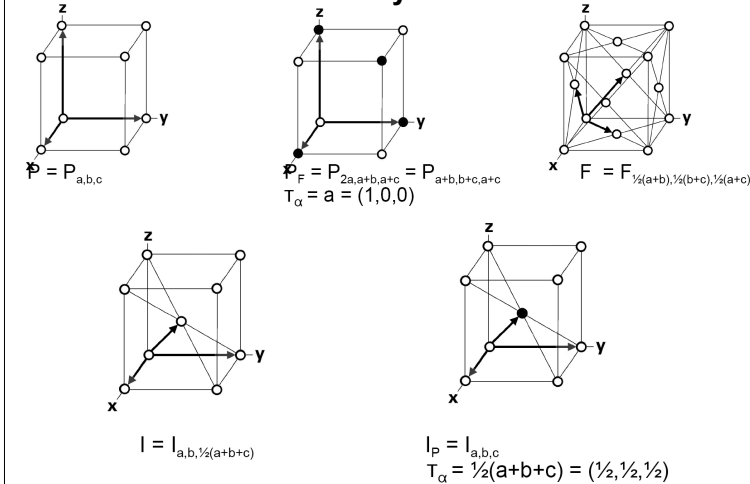
trigonal system



hexagonal system

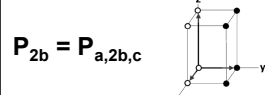


MAGNETIC SPACE GROUP LATTICES cubic system



Magnetic Space Group
Type IIIb, M_R , Example $P_{2b}c'a'2_1$ (No. 29.7.204)

$$F = Pca2_1 = T + T(m_x|1/2,0,1/2) + T(m_y|1/2,0,0) + T(2_z|0,0,1/2)$$



$$P_{2b} = P_{a,2b,c}$$

$$t_\alpha = b = (0,1,0)$$

$$D = Pca2_1 = T^D + T^D(m_x|1/2,1,1/2) + T^D(m_y|1/2,1,0) + T^D(2_z|0,0,1/2)$$

If it is primed in the Opechowski-Guccione symbol then it appears in D coupled with t_α , and primed in $(F|D)1'$.

If it is unprimed in the Opechowski-Guccione symbol then it appears unchanged in D, and coupled with t_α and primed in $(F|D)1'$.

$$M_R = T^D(1|0,0,0) + T^D(m_x|1/2,1,1/2) + T^D(m_y|1/2,1,0) + T^D(2_z|0,0,1/2) + T^D(1|0,0,0)' + T^D(m_x|1/2,0,1/2)' + T^D(m_y|1/2,0,0)' + T^D(2_z|0,1,1/2)'$$

TRICLINIC SYSTEM			(1 0,0,0)		
1.1.1	P1				
1.2.2	P11'				
1.3.3	$P_{2b}1$	P1	(0,0,0)		
2.1.4	P1				
2.2.5	P11'				
2.3.6	P1'	P1	(0,0,0)		
2.4.7	$P_{2b}1'$	P1'	(0,0,0)		
MONOCLINIC SYSTEM					
3.1.8	P2				
3.2.9	P21'				
3.3.10	P2'	P1	(0,0,0;a,b,c)	(1 0,0,0)	(2_z 0,0,0)'
3.4.11	$P_{2b}2$	P2	(0,0,0;2a,b,c)	(1 0,0,0)	(2_z 0,0,0)
3.5.12	$P_{2b}2'$	P2'	(0,0,0;a,2b,c)	(1 0,0,0)	(2_z 0,0,0)
3.6.13	P2	C2	(0,0,0;2a,2b,c)	(1 0,0,0)	(2_z 0,0,0)
3.7.14	$P_{2b}2'$	P2'	(0,0,0;a,2b,c)	(1 0,0,0)	(2_z 0,1,0)

N1.N2.N3, where N1 is a sequence number for the group type to which F belongs, numbered the same as given in the International Tables. N2 is a sequence number of the magnetic space group types of the superfamily of F. Group types F always have the assigned number N1.1.N3, and group types F1' the assigned number N1.2.N3. N3 is a global sequential numbering of the magnetic space group types.

15.1.92	C2/c		(1 0,0,0)	(2_z 0,0,1/2)	(1 0,0,0)	(m_y 0,0,1/2)
15.2.93	C2/c1'					
15.3.94	C2'/c	Cc	(0,0,0;a,b,c)			
15.4.95	C2/c'	C2	(0,0,1/4;a,b,c)	(1 0,0,0)	(2_z 0,0,1/2)	(1 0,0,0)'
15.5.96	C2'/c'	P1	(0,0,0;b,(a+b)/2,c)	(1 0,0,0)	(2_z 0,0,1/2)'	(1 0,0,0)
15.6.97	$C_{2b}2/c$	P2/c	(0,0,0;a,b,c)	(1 0,0,0)	(2_z 0,0,1/2)	(1 0,0,0)
15.7.98	$C_{2b}2'/c$	P2'/c	(1/4,1/4,0;a,b,c)	(1 0,0,0)	(2_z 1/2,1/2,1/2)	(1 1/2,1/2,0)
ORTHORHOMBIC SYSTEM						
16.1.99	P222			(1 0,0,0)	(2_z 0,0,0)	(2_z 0,0,0)
16.2.100	P2221'					
16.3.101	P2'2'2'	P2	(0,0,0;b,c,a)	(1 0,0,0)	(2_z 0,0,0)'	(2_z 0,0,0)'
16.4.102	$P_{2b}222$	P222	(0,0,0;2a,b,c)	(1 0,0,0)	(2_z 0,0,0)	(2_z 0,0,0)
16.5.103	$P_{2b}222'$	C222	(0,0,0;2a,2b,c)	(1 0,0,0)	(2_z 0,0,0)	(2_z 0,0,0)
16.6.104	$P_{2b}222'$	F222	(0,0,0;2a,2b,2c)	(1 0,0,0)	(2_z 0,0,0)	(2_z 0,0,0)
16.7.105	$P_{2b}222'$	P222,	(0,0,0;a,b,2c)	(1 0,0,0)	(2_z 0,0,0)	(2_z 0,0,1)

Opechowski-Guccione symbol of the magnetic space group type, based on F.

74.4.653	Imma'	Imm2	(0,1/4,0;a,b,c)	(1 0,0,0)	(2_z 0,0,0)'	(2_z 0,1/2,0)'	(2_z 0,1/2,0)
74.5.654	Im'm'a	C2/c	(0,0,0;a+b,c,b)	(1 0,0,0)	(2_z 0,0,0)'	(2_z 0,1/2,0)'	(2_z 0,1/2,0)
74.6.655	Imm'a'	C2/m	(0,0,0;a+b,a,c)	(1 0,0,0)	(2_z 0,0,0)'	(2_z 0,1/2,0)'	(2_z 0,1/2,0)
74.7.656	Im'm'a'	I2,2,2,	(0,0,1/4;a,b,c)	(1 0,0,0)	(2_z 0,0,0)'	(2_z 0,1/2,0)'	(2_z 0,1/2,0)
74.8.657	$I_{2b}mma$	Pmma	(0,0,0;b,a,c)	(1 0,0,0)	(2_z 0,0,0)	(2_z 0,1/2,0)	(2_z 0,1/2,0)
74.9.658	$I_{2b}m'm'a$	Pnna	(0,0,0;b,a,c)	(1 0,0,0)	(2_z 1/2,1/2,1/2)	(2_z 1/2,0,1/2)	(2_z 0,1/2,0)
74.10.659	$I_{2b}m'm'a'$	Pmna	(0,0,0;a,b,c)	(1 0,0,0)	(2_z 0,0,0)	(2_z 1/2,0,1/2)	(2_z 1/2,0,1/2)
74.11.660	$I_{2b}m'm'a'$	Pnna	(0,0,0;a,b,c)	(1 0,0,0)	(2_z 1/2,1/2,1/2)	(2_z 1/2,0,1/2)	(2_z 1/2,0,1/2)
TETRAGONAL SYSTEM							
75.1.661	P4			(1 0,0,0)	(4_z 0,0,0)	(2_z 0,0,0)	(4_z' 0,0,0)
75.2.662	P41'						
75.3.663	P4'	P2	(0,0,0;b,c,a)	(1 0,0,0)	(4_z 0,0,0)'	(2_z 0,0,0)	(4_z' 0,0,0)'
75.4.664	$P_{2b}4$	P4	(0,0,0;a,b,2c)	(1 0,0,0)	(4_z 0,0,0)	(2_z 0,0,0)	(4_z' 0,0,0)

group type of the subgroup D of index two of F

83.5.707	P4/m'	P4	(0,0,0;a,b,c)	$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 0,0,0)$
83.6.708	P ₂ 4/m	P4/m	(0,0,0;a,b,2c)	$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 0,0,0)$
83.7.709	P ₄ 4/m	P4/m	(0,0,0;a-b,a+b,c)	$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 0,0,0)$
83.8.710	P ₄ 4/m	P4/m	(0,0,0;a-b,a+b,2c)	$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 0,0,0)$
83.9.711	P ₂ 4'/m	P4 ₂ /m	(0,0,0;a,b,2c)	$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,1)$ $(\bar{4}_2 0,0,1)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,1)$ $(\bar{4}_2^{-1} 0,0,1)$
83.10.712	P ₄ 4/m'	P4/n	(1/2,1/2,0;a-b,a+b,c)	$(1 0,0,0)$ $(\bar{1} 1,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 1,0,0)$	$(2_1 0,0,0)$ $(m_1 1,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 1,0,0)$
84.1.713	P4₂/m			$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,1/2)$ $(\bar{4}_2 0,0,1/2)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,1/2)$ $(\bar{4}_2^{-1} 0,0,1/2)$
84.2.714	P4 ₂ /m1'						
84.3.715	P4 ₂ /m	P2/m	(0,0,0;b,c,a)	$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,1/2)$ $(\bar{4}_2 0,0,1/2)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,1/2)$ $(\bar{4}_2^{-1} 0,0,1/2)$
84.4.716	P4 ₂ /m'	P4 ₂	(0,0,0;a,b,c)	$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,1/2)$ $(\bar{4}_2 0,0,1/2)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,1/2)$ $(\bar{4}_2^{-1} 0,0,1/2)$
84.5.717	P4 ₂ '/m'	P4	(0,0,1/4;a,b,c)	$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,1/2)$ $(\bar{4}_2 0,0,1/2)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,1/2)$ $(\bar{4}_2^{-1} 0,0,1/2)$

Origin change and orientation of D with respect to F

86.4.730	P4 ₂ /n'	P4 ₂	(1/2,0,0;a,b,c)	$(1 0,0,0)$ $(\bar{1} 1/2,1/2,1/2)$	$(4_2 1/2,1/2,1/2)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 1/2,1/2,1/2)$	$(4_2^{-1} 1/2,1/2,1/2)$ $(\bar{4}_2^{-1} 0,0,0)$
86.5.731	P4 ₂ '/n'	P4	(0,0,0;a,b,c)	$(1 0,0,0)$ $(\bar{1} 1/2,1/2,1/2)$	$(4_2 1/2,1/2,1/2)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 1/2,1/2,1/2)$	$(4_2^{-1} 1/2,1/2,1/2)$ $(\bar{4}_2^{-1} 0,0,0)$
86.6.732	P4 ₂ /n	I4 _{1/a}	(0,0,0;a-b,a+b,2c)	$(1 0,0,0)$ $(\bar{1} 1/2,1/2,1/2)$	$(4_2 1/2,1/2,1/2)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 1/2,1/2,1/2)$	$(4_2^{-1} 1/2,1/2,1/2)$ $(\bar{4}_2^{-1} 0,0,0)$
87.1.733	I4/m			$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 0,0,0)$
87.2.734	I4/m1'						
87.3.735	I4'/m	C2/m	(0,0,0;a+b,c,a)	$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 0,0,0)$
87.				$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 0,0,0)$
87.				$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 0,0,0)$
87.				$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 0,0,0)$ $(\bar{4}_2 0,0,0)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 0,0,0)$
87.				$(1 0,0,0)$ $(\bar{1} 0,0,0)$	$(4_2 1/2,1/2,1/2)$ $(\bar{4}_2 1/2,1/2,1/2)$	$(2_1 0,0,0)$ $(m_1 0,0,0)$	$(4_2^{-1} 1/2,1/2,1/2)$ $(\bar{4}_2^{-1} 1/2,1/2,1/2)$
87.8.740	I ₄ 4/m'	P4/n	(1/2,0,1/4;a,b,c)	$(1 0,0,0)$ $(\bar{1} 1/2,1/2,1/2)$	$(4_2 0,0,0)$ $(\bar{4}_2 1/2,1/2,1/2)$	$(2_1 0,0,0)$ $(m_1 1/2,1/2,1/2)$	$(4_2^{-1} 0,0,0)$ $(\bar{4}_2^{-1} 1/2,1/2,1/2)$

Coset representatives of the decomposition of the magnetic space group with respect to its translational subgroup.

Recognizing the different space group types, Type I, uncolored space groups							
29.5.202	Pc'a'2	P2 ₁	(0,0,0;b,c,a)	$(1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(m_1 1/2,0,0)$	$(2_1 0,0,1/2)$
29.6.203	P ₂ ca'	P2					$(2_1 0,0,1/2)$
29.7.204	P ₂ c'a'	P2					$(2_1 0,0,1/2)$
30.1.205	Pnc2			$(1 0,0,0)$	$(m_1 0,1/2,1/2)$	$(m_1 0,1/2,1/2)$	$(2_1 0,0,0)$
30.2.206	Pnc21'						
30.3.207	Pn'c2'	Pc	(0,1/4,0;a,b,c)				$(2_1 0,0,0)$
30.4.208	Pnc2'	Pc	(0,0,0;c,a,b+c)				$(2_1 0,0,0)$
30.5.209	Pn'c'2	P2	(0,0,0;b,c,a)	$(1 0,0,0)$	$(m_1 0,1/2,1/2)$	$(m_1 0,1/2,1/2)$	$(2_1 0,0,0)$
30.6.210	P ₂ nc2	Pnc2	(0,0,0;2a,b,c)	$(1 0,0,0)$	$(m_1 0,1/2,1/2)$	$(m_1 0,1/2,1/2)$	$(2_1 0,0,0)$
30.7.211	P ₂ nc2'	Pnn2	(1/2,0,0;2a,b,c)	$(1 0,0,0)$	$(m_1 0,1/2,1/2)$	$(m_1 1/2,1/2,1/2)$	$(2_1 1,0,0)$
31.1.212	Pmn2₁			$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$
31.2.213	Pmn2 ₁ '						
31.3.214	Pmn2 ₁ '	Pc	(0,0,0;a,b,a+c)	$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$
31.4.215	Pmn'2 ₁ '	Pm	(0,0,0;b,ā,c)	$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$
31.5.216	Pm'n'2 ₁	P2 ₁	(1/4,0,0;b,c,a)	$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$
31.6.217	P ₂ mn2 ₁	Pmn2 ₁	(0,0,0;a,2b,c)	$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$

First entry for each family in blue is the regular uncolored space group

Recognizing the different space group types, Type II, grey groups							
29.5.202	Pc'a'2	P2 ₁	(0,0,0;b,c,a)	$(1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(m_1 1/2,0,0)$	$(2_1 0,0,1/2)$
29.6.203	P ₂ ca'	P2					$(2_1 0,0,1/2)$
29.7.204	P ₂ c'a'	P2					$(2_1 0,0,1/2)$
30.1.205	Pnc2			$(1 0,0,0)$	$(m_1 0,1/2,1/2)$	$(m_1 0,1/2,1/2)$	$(2_1 0,0,0)$
30.2.206	Pnc21'						
30.3.207	Pn'c2'	Pc	(0,1/4,0;a,b,c)	$(1 0,0,0)$	$(m_1 0,1/2,1/2)$	$(m_1 0,1/2,1/2)$	$(2_1 0,0,0)$
30.4.208	Pnc2'	Pc					$(2_1 0,0,0)$
30.5.209	Pn'c'2	P2					$(2_1 0,0,0)$
30.6.210	P ₂ nc2	Pnc2					$(2_1 0,0,0)$
30.7.211	P ₂ nc2'	Pnn2					$(2_1 1,0,0)$
31.1.212	Pmn2₁			$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$
31.2.213	Pmn2₁'						
31.3.214	Pmn2 ₁ '	Pc	(0,0,0;a,b,a+c)	$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$
31.4.215	Pmn'2 ₁ '	Pm	(0,0,0;b,ā,c)	$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$
31.5.216	Pm'n'2 ₁	P2 ₁	(1/4,0,0;b,c,a)	$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$
31.6.217	P ₂ mn2 ₁	Pmn2 ₁	(0,0,0;a,2b,c)	$(1 0,0,0)$	$(m_1 0,0,0)$	$(m_1 1/2,0,1/2)$	$(2_1 1/2,0,1/2)$

Second entry for each family is the grey space group. The symbol is the same as the uncolored group followed by 1'.

Numbering	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
29.5.202	$Pc'a2_1$	$P2_1$	(0,0,0;b,c,a)	(1 0,0,0)	$(m_x 1/2,0,1/2)'$	$(m_y 1/2,0,0)'$	$(2_z 0,0,1/2)$	
29.6.203	$P_{2b}c'a$						$(2_z 0,0,1/2)$	
29.7.204	$P_{2b}c'a$						$(2_z 0,0,1/2)$	
Recognizing the different space group types, Type IIIa, M_T (no anti-translations)								
30.1.205	$Pnc2$			(1 0,0,0)	$(m_x 0,1/2,1/2)$	$(m_y 0,1/2,1/2)$	$(2_z 0,0,0)$	
30.2.206	$Pnc21'$							
30.3.207	$Pn'c2'$	Pc	(0,1/4,0;a,b,c)	(1 0,0,0)	$(m_x 0,1/2,1/2)'$	$(m_y 0,1/2,1/2)$	$(2_z 0,0,0)'$	
30.4.208	$Pnc2''$	Pc	(0,0,0;c,a,b+c)	(1 0,0,0)	$(m_x 0,1/2,1/2)$	$(m_y 0,1/2,1/2)'$	$(2_z 0,0,0)'$	
30.5.209	$Pn'c2'$	P2	(0,0,0;b,c,a)	(1 0,0,0)	$(m_x 0,1/2,1/2)'$	$(m_y 0,1/2,1/2)'$	$(2_z 0,0,0)$	
30.6.210	$P_{2a}nc2$	Pnc2	(0,0,0;2a,b,c)	(1 0,0,0)	$(m_x 0,1/2,1/2)$	$(m_y 0,1/2,1/2)$	$(2_z 0,0,0)$	
30.7.211	$P_{2a}nc2'$	Pnn2	(1/2,0,0;2a,b,c)	(1 0,0,0)	$(m_x 0,1/2,1/2)$	$(m_y 1/2,1/2)$	$(2_z 1,0,0)$	
Entries with primed coset representatives								
31.1.212	$Pmn2_1$						$(2_z 1/2,0,1/2)$	
31.2.213	$Pmn2_1'$							
31.3.214	$Pm'n2_1'$	Pc	(0,0,0;a,b,a+c)	(1 0,0,0)	$(m_x 0,0,0)'$	$(m_y 1/2,0,1/2)$	$(2_z 1/2,0,1/2)'$	
31.4.215	$Pm'n2_1'$	Pm	(0,0,0;b, \bar{a} ,c)	(1 0,0,0)	$(m_x 0,0,0)$	$(m_y 1/2,0,1/2)'$	$(2_z 1/2,0,1/2)'$	
31.5.216	$Pm'n2_1'$	P2 ₁	(1/4,0,0;b,c,a)	(1 0,0,0)	$(m_x 0,0,0)'$	$(m_y 1/2,0,1/2)'$	$(2_z 1/2,0,1/2)'$	
31.6.217	$P_{2a}mn2_1$	Pmn2 ₁	(0,0,0;a,2b,c)	(1 0,0,0)	$(m_x 0,0,0)$	$(m_y 1/2,0,1/2)$	$(2_z 1/2,0,1/2)$	

Numbering	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol	Symbol
29.5.202	$Pc'a2_1$	$P2_1$	(0,0,0;b,c,a)	(1 0,0,0)	$(m_x 1/2,0,1/2)'$	$(m_y 1/2,0,0)'$	$(2_z 0,0,1/2)$	
29.6.203	$P_{2b}c'a$						$(2_z 0,0,1/2)$	
29.7.204	$P_{2b}c'a$						$(2_z 0,0,1/2)$	
Recognizing the different space group types, Type IIIb, M_R (with anti-translations)								
30.1.205	$Pnc2$			(1 0,0,0)	$(m_x 0,1/2,1/2)$	$(m_y 0,1/2,1/2)$	$(2_z 0,0,0)$	
30.2.206	$Pnc21'$							
30.3.207	$Pn'c2'$	Pc	(0,1/4,0;a,b,c)	(1 0,0,0)	$(m_x 0,1/2,1/2)'$	$(m_y 0,1/2,1/2)$	$(2_z 0,0,0)'$	
30.4.208	$Pnc2''$	Pc	(0,0,0;c,a,b+c)	(1 0,0,0)	$(m_x 0,1/2,1/2)$	$(m_y 0,1/2,1/2)'$	$(2_z 0,0,0)'$	
30.5.209	$Pn'c2'$	P2	(0,0,0;b,c,a)	(1 0,0,0)	$(m_x 0,1/2,1/2)'$	$(m_y 0,1/2,1/2)'$	$(2_z 0,0,0)$	
30.6.210	$P_{2a}nc2$	Pnc2	(0,0,0;2a,b,c)	(1 0,0,0)	$(m_x 0,1/2,1/2)$	$(m_y 0,1/2,1/2)$	$(2_z 0,0,0)$	
30.7.211	$P_{2a}nc2'$	Pnn2	(1/2,0,0;2a,b,c)	(1 0,0,0)	$(m_x 0,1/2,1/2)$	$(m_y 1/2,1/2)$	$(2_z 1,0,0)$	
Entries with unprimed coset representatives (and colored lattices)								
31.1.212	$Pmn2_1$						$(2_z 1/2,0,1/2)$	
31.2.213	$Pmn2_1'$							
31.3.214	$Pm'n2_1'$	Pc	(0,0,0;a,b,a+c)	(1 0,0,0)	$(m_x 0,0,0)'$	$(m_y 1/2,0,1/2)$	$(2_z 1/2,0,1/2)'$	
31.4.215	$Pm'n2_1'$	Pm	(0,0,0;b, \bar{a} ,c)	(1 0,0,0)	$(m_x 0,0,0)$	$(m_y 1/2,0,1/2)'$	$(2_z 1/2,0,1/2)'$	
31.5.216	$Pm'n2_1'$	P2 ₁	(1/4,0,0;b,c,a)	(1 0,0,0)	$(m_x 0,0,0)'$	$(m_y 1/2,0,1/2)'$	$(2_z 1/2,0,1/2)'$	
31.6.217	$P_{2a}mn2_1$	Pmn2 ₁	(0,0,0;a,2b,c)	(1 0,0,0)	$(m_x 0,0,0)$	$(m_y 1/2,0,1/2)$	$(2_z 1/2,0,1/2)$	

Typos in Opechowski & Guccione (1965) corrected by Opechowski (1986), given in Litvin (2001)		
Numbering In Table 1	Opechowski & Guccione (1965)	Opechowski (1986)
16.4.102	$P_{2s}222$	$P_{2a}222$
43.4.323	Fdd'2	Fd'd'2
47.6.352	$P_{2s}mmm$	$P_{2a}mmm$
67.17.593	$C_1m'm'a'$	$C_1m'ma'$
108.8.899	I4'cm'	$I_p4'cm'$
108.9.900	I4c'm'	$I_p4c'm'$
124.1.1018	P4/mcr	P4/mcc
132.4.1113	$P4_2/mcm'$	$P4_2'/mcm'$

Other changes to Opechowski-Guccione symbols given by Litvin (2001)		
Numbering In Table 1	Opechowski & Guccione (1965) Opechowski (1986)	Table 1 Litvin (2001)
131.13.1109	$P_P4_2'/m'mc$	$P_P4_2'/m'mc'$
177.7.1385	$P_{2c}6'22$	$P_{2c}6'22'$
180.7.1402	$P_{2c}6_2'22$	$P_{2c}6_2'22'$

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Colored lattice types that cannot be setup with color group option in GSAS

Triclinic: P_{2s}
 Monoclinic: $P_{2a}, P_{2b}, P_{2c}, P_C, C_{2C}$
 Orthorhombic: $P_{2a}, P_{2b}, P_{2c}, P_C, P_F, P_A, A_{2a}, A_I, C_{2C}, C_I$
 Tetragonal: P_{2c}, P_C, 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