Color Symmetry and Magnetic Space Groups

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- ❑History- bicolor symmetry
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- ❑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:

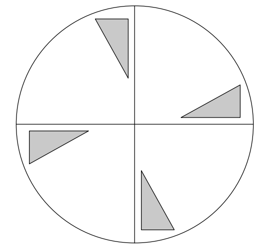
Associativity: For all a, b and c in G, $(a * b) * c = a * (b * c)$.
Identity element: There is an element e in G such that for all a in G, $e * a = a * e = a$.
Inverse element: For all a in G, there is an element b in G such that $a * b = b * a = e$, where e is the identity element from the previous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

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

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



Bicolor Symmetry Groups

1929 Heesch, introduces the antiidentity operation properties: $u^2 = 1$, $ut = tu$ for all $t \in T$
aka time reversal group = {1,1'}

1945 Shubnikov, re-introduces concept

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

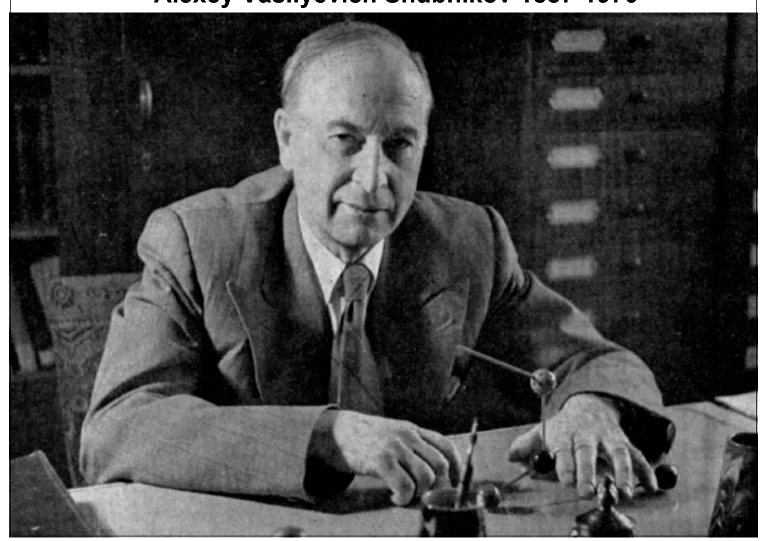
1955 Belov et al., first complete listing of the bicolor space groups

1957 Zamorzaev, group theoretical derivation of bicolor space groups

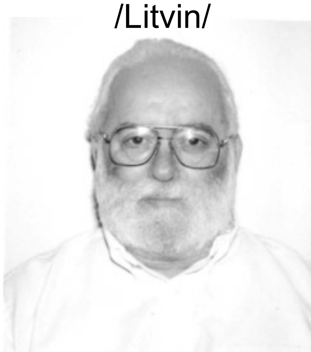
1965 Opechowski and Guccione, first complete derivation and enumeration of the bicolor space groups

2001 Litvin, corrected Opechowski-Guccione symbols

Alexey Vasilyevich Shubnikov 1887-1970



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 ∪ G1’ for some crystallographic point group G

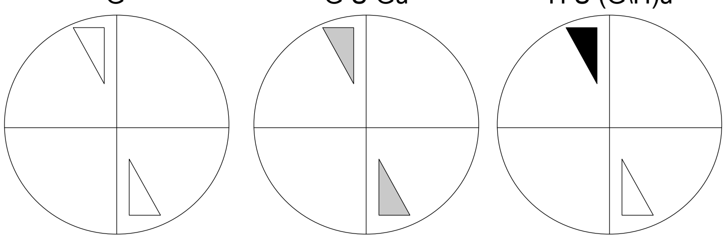
Type III, M = H ∪ (G\H)1’ for some crystallographic point group G, where H is a halving group of G.

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

H	**2 = {1,2}**	**m = {1,m}**	**$\bar{1}$ = {1,i}**
G\H	**{i,m}**	**{2,i}**	**{2,m}**
(G\H)1’	**{i’,m’}**	**{2’,i’}**	**{2’,m’}**
H ∪ (G\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\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	-4’2m’	-42’m’		
4/mmm	4/m’mm	4’/mm’m	4’/m’m’m	4/mm’m’	4/m’m’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/m’mm	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

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

	$^{[010]}2$ 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 ∪ F1’ for some crystallographic space group F
230 grey
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 ∈ *4*.

*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}

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, *T*W denotes the right coset decomposition of *T* in G. The left cosets W*T* 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

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Type III, M = D ∪ (F\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)

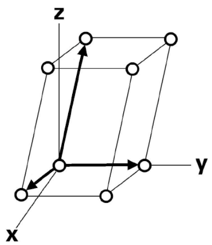
M_T = D + (F\D)1'

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

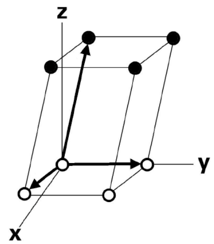
(F\D)1' = T(2_y|0,0,0)' + T(i|0,0,0)'

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



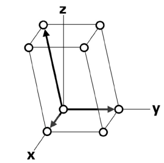
$P = P_{a,b,c}$



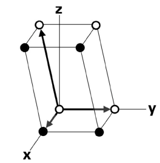
$P_{2s} = P_{a,b,2c}$
$T_\alpha = c = (0,0,1)$

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)

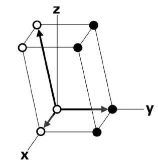
MAGNETIC SPACE GROUP LATTICES
monoclinic system (y is the unique axis)



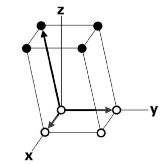
$P = P_{a,b,c}$



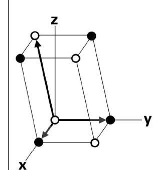
$P_{2a} = P_{2a,b,c}$
$T_\alpha = a = (1,0,0)$



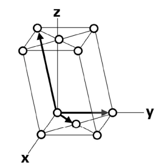
$P_{2b} = P_{a,2b,c}$
$T_\alpha = b = (0,1,0)$



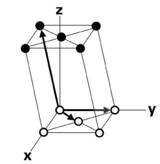
$P_{2c} = P_{a,b,2c}$
$T_\alpha = c = (0,0,1)$



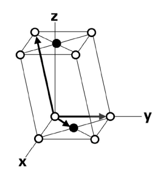
$P_C = P_{2a,a+b,c} = P_{a-b,a+b,c}$
$T_\alpha = a = (1,0,0)$



$C = C_{½(a+b),b,c}$

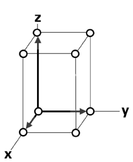


$C_{2c} = C_{½(a+b),b,2c}$
$T_\alpha = c = (0,0,1)$

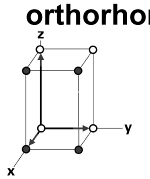


$C_P = C_{a+b,b,c} = C_{a,b,c}$
$T_\alpha = ½(a+b) = (½,½,0)$

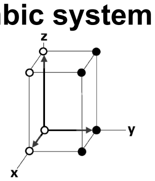
MAGNETIC SPACE GROUP LATTICES
orthorhombic system



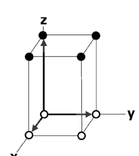
$P = P_{a,b,c}$



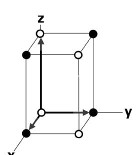
$P_{2a} = P_{2a,b,c}$
$T_\alpha = a = (1,0,0)$



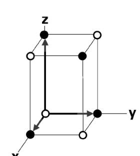
$P_{2b} = P_{a,2b,c}$
$T_\alpha = b = (0,1,0)$



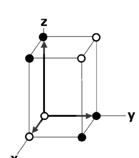
$P_{2c} = P_{a,b,2c}$
$T_\alpha = c = (0,0,1)$



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

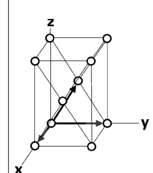


$P_F = P_{2a,a+b,a+c}$
$= P_{a+b,b+c,a+c}$
$T_\alpha = a = (1,0,0)$

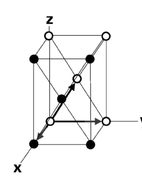


$P_A = P_{a,2b,b+c}$
$T_\alpha = b = (0,1,0)$

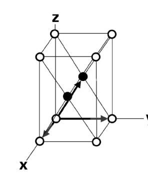
MAGNETIC SPACE GROUP LATTICES
orthorhombic system, continued



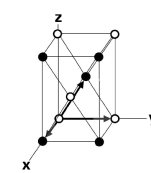
$A = A_{a,b,½(b+c)}$



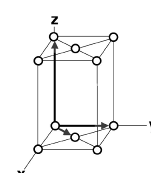
$A_{2a} = A_{2a,b,b+c}$
$T_\alpha = a = (1,0,0)$



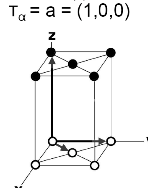
$A_P = A_{a,b,c}$
$T_\alpha = ½(b+c) = (0,½,½)$



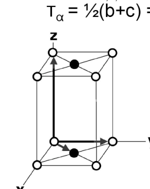
$A_I = A_{2a,b,½(2a+b+c)}$
$T_\alpha = a = (1,0,0)$



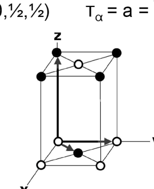
$C = C_{½(a+b),b,c}$



$C_{2c} = C_{½(a+b),b,2c}$
$T_\alpha = c = (0,0,1)$

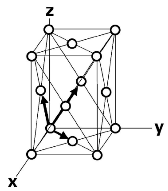


$C_P = C_{a+b,b,c} = C_{a,b,c}$
$T_\alpha = ½(a+b) = (½,½,0)$

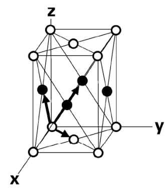


$C_I = C_{a,b,½(a+b+2c)}$
$T_\alpha = c = (0,0,1)$

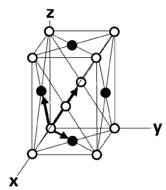
MAGNETIC SPACE GROUP LATTICES
orthorhombic system, continued



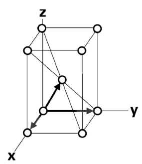
$F = F_{\frac{1}{2}(a+b),\frac{1}{2}(b+c),\frac{1}{2}(a+c)}$



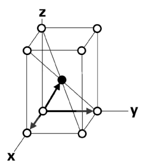
$F_C = F_{\frac{1}{2}(a+b),b,c}$
$T_\alpha = \frac{1}{2}(a+c) = (\frac{1}{2},0,\frac{1}{2})$



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

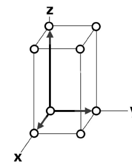


$I = I_{a,b,\frac{1}{2}(a+b+c)}$

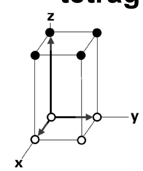


$I_P = I_{a,b,c}$
$T_\alpha = \frac{1}{2}(a+b+c) = (\frac{1}{2},\frac{1}{2},\frac{1}{2})$

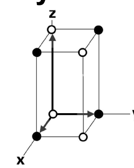
MAGNETIC SPACE GROUP LATTICES
tetragonal system



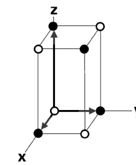
$P = P_{a,b,c}$



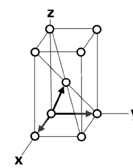
$P_{2c} = P_{a,b,2c}$
$T_\alpha = c = (0,0,1)$



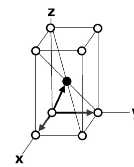
$P_{a-b,a+b}\ (P_C) = P_{a-b,a+b,c}$
$= P_P = P_{2a,a+b,c}$
$T_\alpha = a = (1,0,0)$



$P_I = P_{a-b,a+b,a+c}$
$T_\alpha = a = (1,0,0)$



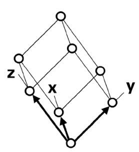
$I = I_{a,b,\frac{1}{2}(a+b+c)}$



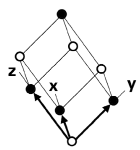
$I_P = I_{a,b,c}$
$T_\alpha = \frac{1}{2}(a+b+c) = (\frac{1}{2},\frac{1}{2},\frac{1}{2})$

MAGNETIC SPACE GROUP LATTICES

trigonal system

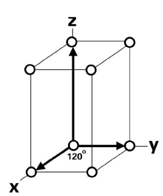


$R = R_{a,b,c}$

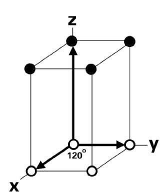


$R_{2a,a+b,a+c} = R_R = R_{a+b,b+c,a+c}$
$T_\alpha = a = (1,0,0)$

hexagonal system

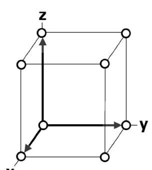


$P = P_{a,b,c}$

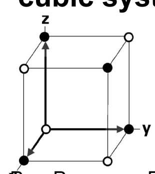


$P_{2c} = P_{a,b,2c}$
$T_\alpha = c = (0,0,1)$

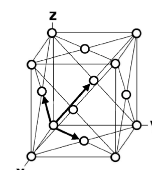
MAGNETIC SPACE GROUP LATTICES
cubic system



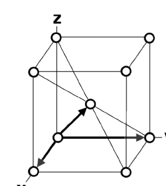
$P = P_{a,b,c}$



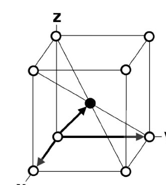
$P_F = P_{2a,a+b,a+c} = P_{a+b,b+c,a+c}$
$T_\alpha = a = (1,0,0)$



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



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

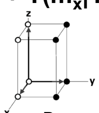


$I_P = I_{a,b,c}$
$T_\alpha = \frac{1}{2}(a+b+c) = (\frac{1}{2},\frac{1}{2},\frac{1}{2})$

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

1.1.1	**P1**			**(1|0,0,0)**	
1.2.2	P11'				
1.3.3	$P_{2s}1$	P1	(0,0[illegible]	[illegible]	
2.1.4	**$P\bar{1}$**			[illegible]	[illegible]
2.2.5	$P\bar{1}1'$				
2.3.6	$P\bar{1}'$	P1	(0,0[illegible]	[illegible]	[illegible]
2.4.7	$P_{2s}\bar{1}$	$P\bar{1}$	(0,0[illegible]	[illegible]	[illegible]

MONOCLINIC SYSTEM

3.1.8	**P2**			[illegible]	[illegible]
3.2.9	P21'				
3.3.10	P2'	P1	(0,0,0;a,b,c)	(1|0,0,0)	$(2_y\|0,0,0)'$
3.4.11	$P_{2a}2$	P2	(0,0,0;2a,b,c)	(1|0,0,0)	$(2_y\|0,0,0)$
3.5.12	$P_{2b}2$	P2	(0,0,0;a,2b,c)	(1|0,0,0)	$(2_y\|0,0,0)$
3.6.13	P_C2	C2	(0,0,0;2a,2b,c)	(1|0,0,0)	$(2_y\|0,0,0)$
3.7.14	$P_{2b}2'$	$P2_1$	(0,0,0;a,2b,c)	(1|0,0,0)	$(2_y\|0,1,0)$

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)**	**$(2_y\|0,0,1/2)$**	**$(\bar{1}\|0,0,0)$**	**$(m_y\|0,0,1/2$**
15.2.93	C2/c1'						
15.3.94	C2'/c	Cc	(0,0,0;a,b,c)	[illegible]	[illegible]	[illegible]	[illegible]
15.4.95	C2/c'	C2	(0,0,1/4;a,b,c)	(1|0,0,0)	$(2_y\|0,0,1/2)$	$(\bar{1}\|0,0,0)'$	$(m_y\|0,0,1/2$
15.5.96	C2'/c'	$P\bar{1}$	(0,0,0;b,{a+b}/2,c)	(1|0,0,0)	$(2_y\|0,0,1/2)'$	$(\bar{1}\|0,0,0)$	$(m_y\|0,0,1/2$
15.6.97	C_P2/c	P2/c	(0,0,0;a,b,c)	(1|0,0,0)	$(2_y\|0,0,1/2)$	$(\bar{1}\|0,0,0)$	$(m_y\|0,0,1/2$
15.7.98	C_P2'/c	$P2_1/c$	(1/4,1/4,0;a,b,c)	(1|0,0,0)	$(2_y\|1/2,1/2,1/2)$	$(\bar{1}\|1/2,1/2,0)$	$(m_y\|0,0,1/2$

ORTHORHOMBIC SYSTEM

16.1.99	**P222**			**(1|0,0,0)**	**$(2_x\|0,0,0)$**	**$(2_y\|0,0,0)$**	**$(2_z\|0,0,0)$**
16.2.100	P2221'						
16.3.101	P2'2'2	P2	(0,0,0;b,c,a)	(1|0,0,0)	$(2_x\|0,0,0)'$	$(2_y\|0,0,0)'$	$(2_z\|0,0,0)$
16.4.102	$P_{2a}222$	P222	(0,0,0;2a,b,c)	(1|0,0,0)	$(2_x\|0,0,0)$	$(2_y\|0,0,0)$	$(2_z\|0,0,0)$
16.5.103	P_C222	C222	(0,0,0;2a,2b,c)	(1|0,0,0)	$(2_x\|0,0,0)$	$(2_y\|0,0,0)$	$(2_z\|0,0,0)$
16.6.104	P_F222	F222	(0,0,0;2a,2b,2c)	(1|0,0,0)	$(2_x\|0,0,0)$	$(2_y\|0,0,0)$	$(2_z\|0,0,0)$
16.7.105	$P_{2c}22'2'$	$P222_1$	(0,0,0;a,b,2c)	(1|0,0,0)	$(2_x\|0,0,0)$	$(2_y\|0,0,1)$	$(2_z\|0,0,1)$

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) $(\bar{1}\|0,0,0)'$	$(2_x\|0,0,0)'$ $(m_x\|0,0,0)$	$(2_y\|0,1/2,0)'$ $(m_y\|0,1/2,0)$	$(2_z\|0,1/2,0)$ $(m_z\|0,1/2,0)'$
74.5.654	Im'm'a	C2/c	$(0,0,0;a+b,c,\bar{b})$	(1|0,0,0) $(\bar{1}\|0$[illegible]	$(2_x\|0,0,0)'$ [illegible]	$(2_y\|0,1/2,0)'$ $(m_y\|0,1/2,0)'$	$(2_z\|0,1/2,0)$ $(m_z\|0,1/2,0)$
74.6.655	Imm'a'	C2/m	$(0,0,0;a+b,\bar{a},c)$	(1|0[illegible] $(\bar{1}\|0$[illegible]	[illegible]	$(2_y\|0,1/2,0)'$ $(m_y\|0,1/2,0)'$	$(2_z\|0,1/2,0)'$ $(m_z\|0,1/2,0)'$
74.7.656	Im'm'a'	$I2_12_12_1$	(0,0,1/4;a,b,c)	(1|0,0,0) $(\bar{1}\|0,0,0)'$	$(2_x\|0,0,0)$ $(m_x\|0,0,0)'$	$(2_y\|0,1/2,0)$ $(m_y\|0,1/2,0)'$	$(2_z\|0,1/2,0)$ $(m_z\|0,1/2,0)'$
74.8.657	I_Pmma	Pmma	$(0,0,0;b,\bar{a},c)$	(1|0,0,0) $(\bar{1}\|0,0,0)$	$(2_x\|0,0,0)$ $(m_x\|0,0,0)$	$(2_y\|0,1/2,0)$ $(m_y\|0,1/2,0)$	$(2_z\|0,1/2,0)$ $(m_z\|0,1/2,0)$
74.9.658	$I_Pm'm'a$	Pnna	$(0,0,0;b,\bar{a},c)$	(1|0,0,0) $(\bar{1}\|0,0,0)$	$(2_x\|1/2,1/2,1/2)$ $(m_x\|1/2,1/2,1/2)$	$(2_y\|1/2,0,1/2)$ $(m_y\|1/2,0,1/2)$	$(2_z\|0,1/2,0)$ $(m_z\|0,1/2,0)$
74.10.659	$I_Pmm'a'$	Pmna	(0,0,0;a,b,c)	(1|0,0,0) $(\bar{1}\|0,0,0)$	$(2_x\|0,0,0)$ $(m_x\|0,0,0)$	$(2_y\|1/2,0,1/2)$ $(m_y\|1/2,0,1/2)$	$(2_z\|1/2,0,1/2)$ $(m_z\|1/2,0,1/2)$
74.11.660	$I_Pm'ma'$	Pnma	(0,0,0;a,b,c)	(1|0,0,0) $(\bar{1}\|0,0,0)$	$(2_x\|1/2,1/2,1/2)$ $(m_x\|1/2,1/2,1/2)$	$(2_y\|0,1/2,0)$ $(m_y\|0,1/2,0)$	$(2_z\|1/2,0,1/2)$ $(m_z\|1/2,0,1/2)$

TETRAGONAL SYSTEM

75.1.661	**P4**			**(1|0,0,0)**	**$(4_z\|0,0,0)$**	**$(2_z\|0,0,0)$**	**$(4_z^{-1}\|0,0,0)$**
75.2.662	P41'						
75.3.663	P4'	P2	(0,0,0;b,c,a)	(1|0,0,0)	$(4_z\|0,0,0)'$	$(2_z\|0,0,0)$	$(4_z^{-1}\|0,0,0)'$
75.4.664	$P_{2c}4$	P4	(0,0,0;a,b,2c)	(1|0,0,0)	$(4_z\|0,0,0)$	$(2_z\|0,0,0)$	$(4_z^{-1}\|0,0,0)$

group type of the subgroup D of index two of F

83.5.707	$P4'/m'$	$P\bar{4}$	(0,0,0;a,b,c)	$(1\|0,0,0)$ $(\bar{1}\|0,0,0)'$	$(4_z\|0,0,0)'$ $(\bar{4}_z\|0,0,0)$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)'$	$(4_z^{-1}\|0,0,0)'$ $(\bar{4}_z^{-1}\|0,0,0)$
83.6.708	$P_{2c}4/m$	$P4/m$	(0,0,0;a,b,2c)	$(1\|0,0,0)$ $(\bar{1}\|0,0,0)$	$(4_z\|0,0,0)$ $(\bar{4}_z\|0,0,0)$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)$	$(4_z^{-1}\|0,0,0)$ $(\bar{4}_z^{-1}\|0,0,0)$
83.7.709	P_P4/m	$P4/m$	(0,0,0;a-b,a+b,c)	$(1\|0,0,0)$ $(\bar{1}\|0,0,$			$(4_z^{-1}\|0,0,0)$ $(\bar{4}_z^{-1}\|0,0,0)$
83.8.710	P_I4/m	$P4/m$	(0,0,0;a-b,a+b,2c)	$(1\|0,0,$ $(\bar{1}\|0,0,$			$(4_z^{-1}\|0,0,0)$ $(\bar{4}_z^{-1}\|0,0,0)$
83.9.711	$P_{2c}4'/m$	$P4_2/m$	(0,0,0;a,b,2c)	$(1\|0,0,0)$ $(\bar{1}\|0,0,0)$	$(4_z\|0,0,1)$ $(\bar{4}_z\|0,0,1)$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)$	$(4_z^{-1}\|0,0,1)$ $(\bar{4}_z^{-1}\|0,0,1)$
83.10.712	P_P4/m'	$P4/n$	(1/2,1/2,0;a-b,a+b,c)	$(1\|0,0,0)$ $(\bar{1}\|1,0,0)$	$(4_z\|0,0,0)$ $(\bar{4}_z\|1,0,0)$	$(2_z\|0,0,0)$ $(m_z\|1,0,0)$	$(4_z^{-1}\|0,0,0)$ $(\bar{4}_z^{-1}\|1,0,0)$
84.1.713	$P4_2/m$			$(1\|0,0,0)$ $(\bar{1}\|0,0,0)$	$(4_z\|0,0,1/2)$ $(\bar{4}_z\|0,0,1/2)$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)$	$(4_z^{-1}\|0,0,1/2)$ $(\bar{4}_z^{-1}\|0,0,1/2)$
84.2.714	$P4_2/m1'$						
84.3.715	$P4_2'/m$	$P2/m$	(0,0,0;b,c,a)	$(1\|0,0,0)$ $(\bar{1}\|0,0,0)$	$(4_z\|0,0,1/2)'$ $(\bar{4}_z\|0,0,1/2)'$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)$	$(4_z^{-1}\|0,0,1/2)'$ $(\bar{4}_z^{-1}\|0,0,1/2)'$
84.4.716	$P4_2/m'$	$P4_2$	(0,0,0;a,b,c)	$(1\|0,0,0)$ $(\bar{1}\|0,0,0)'$	$(4_z\|0,0,1/2)$ $(\bar{4}_z\|0,0,1/2)'$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)'$	$(4_z^{-1}\|0,0,1/2)$ $(\bar{4}_z^{-1}\|0,0,1/2)'$
84.5.717	$P4_2'/m'$	$P\bar{4}$	(0,0,1/4;a,b,c)	$(1\|0,0,0)$ $(\bar{1}\|0,0,0)'$	$(4_z\|0,0,1/2)'$ $(\bar{4}_z\|0,0,1/2)$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)'$	$(4_z^{-1}\|0,0,1/2)'$ $(\bar{4}_z^{-1}\|0,0,1/2)$

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)	$(1\|0,0,0)$ $(\bar{1}\|1/2,1/2,1/2)'$	$(4_z\|1/2,1/2,1/2)$ $(\bar{4}_z\|0,0,0)'$	$(2_z\|0,0,0)$ $(m_z\|1/2,1/2,1/2)'$	$(4_z^{-1}\|1/2,1/2,1/2)$ $(\bar{4}_z^{-1}\|0,0,0)'$
86.5.731	$P4_2'/n'$	$P\bar{4}$	(0,0,0;a,b,c)	$(1\|0,0,0)$ $(\bar{1}\|1/2,1/2,1/2)'$	$(4_z\|1/2,1/2,1/2)'$ $(\bar{4}_z\|0,0,0)$	$(2_z\|0,0,0)$ $(m_z\|1/2,1/2,1/2)'$	$(4_z^{-1}\|1/2,1/2,1/2)'$ $(\bar{4}_z^{-1}\|0,0,0)$
86.6.732	P_I4_2/n	$I4_1/a$	(0,0,0;a-b,a+b,2c)	$(1\|0,0,0)$ $(\bar{1}\|1/2,1/2,1/2)$	$(4_z\|1/2,1/2,1/2)$ $(\bar{4}_z\|0,0,0)$	$(2_z\|0,0,0)$ $(m_z\|1/2,1/2,1/2)$	$(4_z^{-1}\|1/2,1/2,1/2)$ $(\bar{4}_z^{-1}\|0,0,0)$
87.1.733	$I4/m$			$(1\|0,0,0)$ $(\bar{1}\|0,0,0)$	$(4_z\|0,0,0)$ $(\bar{4}_z\|0,0,0)$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)$	$(4_z^{-1}\|0,0,0)$ $(\bar{4}_z^{-1}\|0,0,0)$
87.2.734	$I4/m1'$						
87.3.735	$I4'/m$	$C2/m$	(0,0,0;a+b,c,a)	$(1\|0,0,0)$ $(\bar{1}\|0,0,0)$	$(4_z\|0,0,0)'$ $(\bar{4}_z\|0,0,0)'$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)$	$(4_z^{-1}\|0,0,0)'$ $(\bar{4}_z^{-1}\|0,0,0)'$
87.				$(1\|0,0,0)$ $(\bar{1}\|0,0,0)'$	$(4_z\|0,0,0)$ $(\bar{4}_z\|0,0,0)'$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)'$	$(4_z^{-1}\|0,0,0)$ $(\bar{4}_z^{-1}\|0,0,0)'$
87.				$(1\|0,0,0)$ $(\bar{1}\|0,0,0)'$	$(4_z\|0,0,0)'$ $(\bar{4}_z\|0,0,0)$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)'$	$(4_z^{-1}\|0,0,0)'$ $(\bar{4}_z^{-1}\|0,0,0)$
87.				$(1\|0,0,0)$ $(\bar{1}\|0,0,0)$	$(4_z\|0,0,0)$ $(\bar{4}_z\|0,0,0)$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)$	$(4_z^{-1}\|0,0,0)$ $(\bar{4}_z^{-1}\|0,0,0)$
87.				$(1\|0,0,0)$ $(\bar{1}\|0,0,0)$	$(4_z\|1/2,1/2,1/2)$ $(\bar{4}_z\|1/2,1/2,1/2)$	$(2_z\|0,0,0)$ $(m_z\|0,0,0)$	$(4_z^{-1}\|1/2,1/2,1/2)$ $(\bar{4}_z^{-1}\|1/2,1/2,1/2)$
87.8.740	I_P4/m'	$P4/n$	(1/2,0,1/4;a,b,c)	$(1\|0,0,0)$ $(\bar{1}\|1/2,1/2,1/2)'$	$(4_z\|0,0,0)$ $(\bar{4}_z\|1/2,1/2,1/2)'$	$(2_z\|0,0,0)$ $(m_z\|1/2,1/2,1/2)'$	$(4_z^{-1}\|0,0,0)$ $(\bar{4}_z^{-1}\|1/2,1/2,1/2)'$

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	$Pc'a'2_1$	$P2_1$	(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	$P_{2b}ca$						$(2_z\|0,0,1/2)$
29.7.204	$P_{2b}c'a$						$(2_z\|0,0,1/2)$
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)				
30.4.208	$Pnc'2'$	Pc	(0,0,0;c,a,b+c)				
30.5.209	$Pn'c'2$	$P2$	(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	$P_{2a}nc'2'$	$Pnn2$	(1/2,0,0;2a,b,c)	$(1\|0,0,0)$	$(m_x\|0,1/2,1/2)$	$(m_y\|1\ 1/2\ 1/2)$	$(2_z\|1,0,0)$
31.1.212	$Pmn2_1$			$(1\|0,0,0)$	$(m_x\|0,0,0)$	$(m_y\|1/2,0,1/2)$	$(2_z\|1/2,0,1/2)$
31.2.213	$Pmn2_11'$						
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	$Pmn'2_1'$	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	$Pm'n'2_1$	$P2_1$	(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	$P_{2b}mn2_1$	$Pmn2_1$	(0,0,0;a,2b,c)	$(1\|0,0,0)$	$(m_x\|0,0,0)$	$(m_y\|1/2,0,1/2)$	$(2_z\|1/2,0,1/2)$

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	$Pc'a'2_1$	$P2_1$	(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						$(2_z\|0,0,1/2)$
29.7.204	P						$(2_z\|0,0,1/2)$
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	$Pnc'2'$	Pc				1/2)'	$(2_z\|0,0,0)'$
30.5.209	$Pn'c'2$	$P2$				1/2)'	$(2_z\|0,0,0)$
30.6.210	$P_{2a}nc2$	$Pnc2$				1/2)	$(2_z\|0,0,0)$
30.7.211	$P_{2a}nc'2'$	$Pnn2$				1/2)	$(2_z\|1,0,0)$
31.1.212	$Pmn2_1$			$(1\|0,0,0)$	$(m_x\|0,0,0)$	$(m_y\|1/2,0,1/2)$	$(2_z\|1/2,0,1/2)$
31.2.213	$Pmn2_11'$						
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	$Pmn'2_1'$	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	$Pm'n'2_1$	$P2_1$	(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	$P_{2b}mn2_1$	$Pmn2_1$	(0,0,0;a,2b,c)	$(1\|0,0,0)$	$(m_x\|0,0,0)$	$(m_y\|1/2,0,1/2)$	$(2_z\|1/2,0,1/2)$

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

Recognizing the different space group types, Type IIIa, M_T (no anti-translations)

29.5.202	$Pc'a'2_1$	$P2_1$	(0,0,0;b,c,a)	$(1\vert 0,0,0)$	$(m_x\vert 1/2,0,1/2)'$	$(m_y\vert 1/2,0,0)'$	$(2_z\vert 0,0,1/2)$
29.6.203	$P_{2b}ca$						$(2_z\vert 0,0,1/2)$
29.7.204	$P_{2b}c'a$						$(2_z\vert 0,0,1/2)$
30.1.205	**Pnc2**			$\mathbf{(1\vert 0,0,0)}$	$\mathbf{(m_x\vert 0,1/2,1/2)}$	$\mathbf{(m_y\vert 0,1/2,1/2)}$	$\mathbf{(2_z\vert 0,0,0)}$
30.2.206	Pnc21'						
30.3.207	Pn'c2'	Pc	(0,1/4,0;a,b,c)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)'$	$(m_y\vert 0,1/2,1/2)$	$(2_z\vert 0,0,0)'$
30.4.208	Pnc'2'	Pc	(0,0,0;c,a,b+c)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)$	$(m_y\vert 0,1/2,1/2)'$	$(2_z\vert 0,0,0)'$
30.5.209	Pn'c'2	P2	(0,0,0;b,c,a)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)'$	$(m_y\vert 0,1/2,1/2)'$	$(2_z\vert 0,0,0)$
30.6.210	$P_{2a}nc2$	Pnc2	(0,0,0;2a,b,c)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)$	$(m_y\vert 0,1/2,1/2)$	$(2_z\vert 0,0,0)$
30.7.211	$P_{2a}nc'2'$	Pnn2	(1/2,0,0;2a,b,c)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)$	$(m_y\vert 1\ 1/2\ 1/2)$	$(2_z\vert 1,0,0)$
31.1.212	$\mathbf{Pmn2_1}$						$\mathbf{(2_z\vert 1/2,0,1/2)}$
31.2.213	$Pmn2_11'$						
31.3.214	$Pm'n2_1'$	Pc	(0,0,0;a,b,a+c)	$(1\vert 0,0,0)$	$(m_x\vert 0,0,0)'$	$(m_y\vert 1/2,0,1/2)$	$(2_z\vert 1/2,0,1/2)'$
31.4.215	$Pmn'2_1'$	Pm	(0,0,0;b,$\bar{a}$,c)	$(1\vert 0,0,0)$	$(m_x\vert 0,0,0)$	$(m_y\vert 1/2,0,1/2)'$	$(2_z\vert 1/2,0,1/2)'$
31.5.216	$Pm'n'2_1$	$P2_1$	(1/4,0,0;b,c,a)	$(1\vert 0,0,0)$	$(m_x\vert 0,0,0)'$	$(m_y\vert 1/2,0,1/2)'$	$(2_z\vert 1/2,0,1/2)$
31.6.217	$P_{2b}mn2_1$	$Pmn2_1$	(0,0,0;a,2b,c)	$(1\vert 0,0,0)$	$(m_x\vert 0,0,0)$	$(m_y\vert 1/2,0,1/2)$	$(2_z\vert 1/2,0,1/2)$

Entries with primed coset representatives

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

29.5.202	$Pc'a'2_1$	$P2_1$	(0,0,0;b,c,a)	$(1\vert 0,0,0)$	$(m_x\vert 1/2,0,1/2)'$	$(m_y\vert 1/2,0,0)'$	$(2_z\vert 0,0,1/2)$
29.6.203	$P_{2b}ca$						$(2_z\vert 0,0,1/2)$
29.7.204	$P_{2b}c'a$						$(2_z\vert 0,0,1/2)$
30.1.205	**Pnc2**			$\mathbf{(1\vert 0,0,0)}$	$\mathbf{(m_x\vert 0,1/2,1/2)}$	$\mathbf{(m_y\vert 0,1/2,1/2)}$	$\mathbf{(2_z\vert 0,0,0)}$
30.2.206	Pnc21'						
30.3.207	Pn'c2'	Pc	(0,1/4,0;a,b,c)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)'$	$(m_y\vert 0,1/2,1/2)$	$(2_z\vert 0,0,0)'$
30.4.208	Pnc'2'	Pc	(0,0,0;c,a,b+c)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)$	$(m_y\vert 0,1/2,1/2)'$	$(2_z\vert 0,0,0)'$
30.5.209	Pn'c'2	P2	(0,0,0;b,c,a)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)'$	$(m_y\vert 0,1/2,1/2)'$	$(2_z\vert 0,0,0)$
30.6.210	$P_{2a}nc2$	Pnc2	(0,0,0;2a,b,c)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)$	$(m_y\vert 0,1/2,1/2)$	$(2_z\vert 0,0,0)$
30.7.211	$P_{2a}nc'2'$	Pnn2	(1/2,0,0;2a,b,c)	$(1\vert 0,0,0)$	$(m_x\vert 0,1/2,1/2)$	$(m_y\vert 1\ 1/2\ 1/2)$	$(2_z\vert 1,0,0)$
31.1.212	$\mathbf{Pmn2_1}$						$\mathbf{(2_z\vert 1/2,0,1/2)}$
31.2.213	$Pmn2_11'$						
31.3.214	$Pm'n2_1'$	Pc	(0,0,0;a,b,a+c)				$(2_z\vert 1/2,0,1/2)'$
31.4.215	$Pmn'2_1'$	Pm	(0,0,0;b,$\bar{a}$,c)				$(2_z\vert 1/2,0,1/2)'$
31.5.216	$Pm'n'2_1$	$P2_1$	(1/4,0,0;b,c,a)	$(1\vert 0,0,0)$	$(m_x\vert 0,0,0)'$	$(m_y\vert 1/2,0,1/2)'$	$(2_z\vert 1/2,0,1/2)$
31.6.217	$P_{2b}mn2_1$	$Pmn2_1$	(0,0,0;a,2b,c)	$(1\vert 0,0,0)$	$(m_x\vert 0,0,0)$	$(m_y\vert 1/2,0,1/2)$	$(2_z\vert 1/2,0,1/2)$

Entries with unprimed coset representatives (and colored lattices)

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	$C_I m'm'a'$	$C_I m'ma'$
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)

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

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